

## UV/Vis/NIR Spectrometer

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## Simple Method of Measuring the Band Gap Energy Value of $\text{TiO}_2$ in the Powder Form using a UV/Vis/NIR Spectrometer

### Introduction

The measurement of the band gap of materials is important in the semiconductor, nanomaterial and solar industries.

This note demonstrates how the band gap of a material can be determined from its UV absorption spectrum.

The term "band gap" refers to the energy difference between the top of the valence band to the bottom of the conduction band (See Figure 1); electrons are able to jump from one band to another. In order for an electron to jump from a valence band to a conduction band, it requires a specific minimum amount of energy for the transition, the band gap energy<sup>1,2</sup>. A diagram illustrating the bandgap is shown in Figure 1.

Measuring the band gap is important in the semiconductor and nanomaterial industries. The band gap energy of insulators is large ( $> 4\text{eV}$ ), but lower for semiconductors ( $< 3\text{eV}$ ). The band gap properties of a semiconductor can be controlled by using different semiconductor alloys such as GaAlAs, InGaAs, and InAlAs. A table of materials and bandgaps is given in Reference 1.

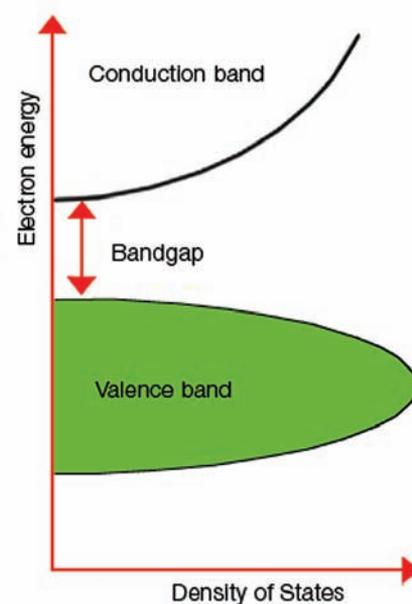


Figure 1. Explanation of band gap.

An alternative strategy is to use layers of different materials coated onto the silicon base material. This is employed in the solar industry in the construction of photovoltaic (PV) solar cells. The bandgap is important as it determines the portion of the solar spectrum a photovoltaic cell absorbs<sup>3</sup>. Much of the solar radiation reaching the Earth is comprised of wavelengths with energies greater than the band gap of silicon. These higher energies will be absorbed by the solar cell, but the difference in energy is converted into heat rather than into usable electrical energy. Consequently, unless the band gap is controlled, the efficiency of the solar cell will be poor. Using layers of different materials with different band gap properties is a proven way to maximize the efficiency of solar cells.

In the semiconductor and nanomaterial industries, titanium dioxide (TiO<sub>2</sub>, commonly known as titania) is added as an ingredient to coatings. TiO<sub>2</sub> is thought to promote the internal trapping of light by scattering (redirecting) the light reflected from the metallic electrode in the active layer and also to improve the transport of charge carriers through the active layer<sup>4</sup>.

### Experimental

It has been found that many of the nanomaterial studies on these materials are being carried out using a small quantity of the sample. Hence, sampling becomes a key issue to this type of analysis. The analysis was carried out using a LAMBDA™ 1050 UV/Vis/NIR spectrometer along with 150-mm integrating sphere (PerkinElmer, Inc., Shelton, CT USA) as shown in Figure 2.



Figure 2. LAMBDA 1050 UV/Vis/NIR System with Integrating Sphere.

This holder (Prima Industries, Mumbai, India – Figure 3) with powder sample in is clamped on the external port of the integrating sphere. A low volume powder sample press was used.



Figure 3. Powder sample press with sample holder.

The optical diagram of the integrating sphere is shown in Figure 4.

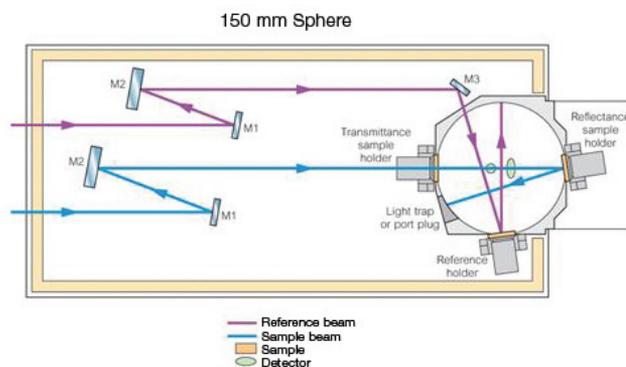


Figure 4. 150-mm Integrating Sphere Optical diagram.

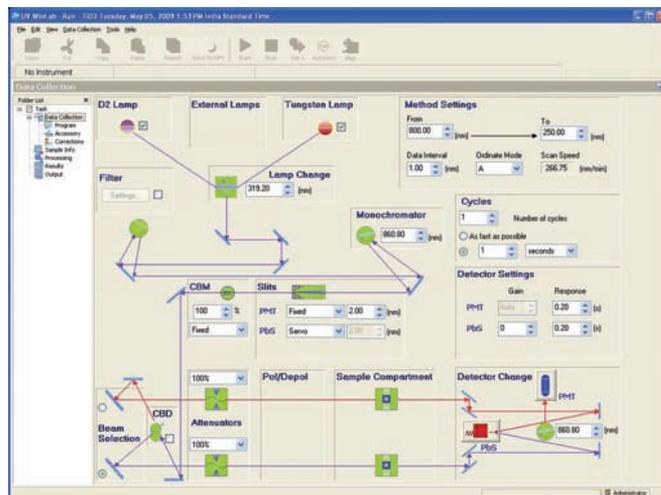


Figure 5. UV WinLab™ Software Setup.

The sample was run using the parameters listed in Table 1.

**Table 1. Instrumental Parameters**

Wavelength Range	250-800 nm
SBW	2 nm
Data Interval	1 nm

The entrance port of the integrating sphere is kept open to minimize the specular reflection component which can cause fringes or noise at the extreme end of the range. The spectra were recorded in absorbance vs. wavelength and % reflectance vs. wavelength modes.

The advantage of using a LAMBDA 1050 was to have a second sample compartment where the integrating sphere can be mounted without blocking the main sample compartment.

### Results and Discussion

The resulting spectrum obtained on TiO<sub>2</sub> is shown in Figure 6.

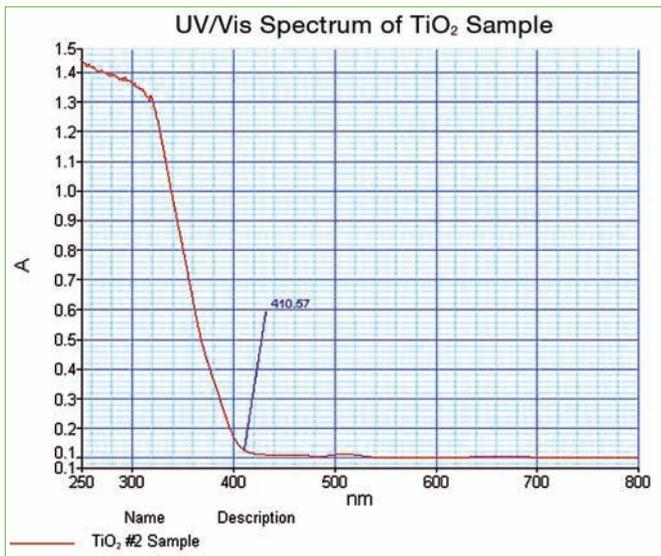


Figure 6. TiO<sub>2</sub> UV/Vis spectrum obtained in this work.

The spectral data recorded showed the strong cut off at 410.57 nm; where the absorbance value is minimum. The data is corroborated in the % Reflectance mode.

### Calculations

$$\text{Band Gap Energy (E)} = h \cdot C / \lambda \quad (1 \ \& \ 3)$$

$$h = \text{Planks constant} = 6.626 \times 10^{-34} \text{ Joules sec}$$

$$C = \text{Speed of light} = 3.0 \times 10^8 \text{ meter/sec}$$

$$\lambda = \text{Cut off wavelength} = 410.57 \times 10^{-9} \text{ meters}$$

H	C	$\lambda$	E	eV
6.63E-34	3.00E+08	4.11E-07	4.84156E-19	3.025976

Where 1eV = 1.6 X 10<sup>-19</sup> Joules (conversion factor)

### Conclusion

With similar experimental conditions and accessories, band gap energy values for various powder nanomaterials can be calculated. With this, the quality of TiO<sub>2</sub> also can be determined. Various other semiconductor nanomaterials can also be subjected to the experiment for which the example spectra from literature are given in Figure 7<sup>5</sup>.

The major advantages of using the specially designed small powder sample holder are:

1. Smaller quantity powder samples can be analyzed directly
2. Due to a specially designed hand press, powder gets caked in the cup firmly and does not slip in to the sphere
3. Sample quantity required is 20-30 times less than the conventional powder sample holder
4. The press gives a very even surface to the sample to conduct reflectance experiments
5. Minimizes the specular component of the reflection as the sample is being exposed directly to the beam.
6. Cost effective sampling device with a depth of 1.5 cm deep and 1 cm diameter.

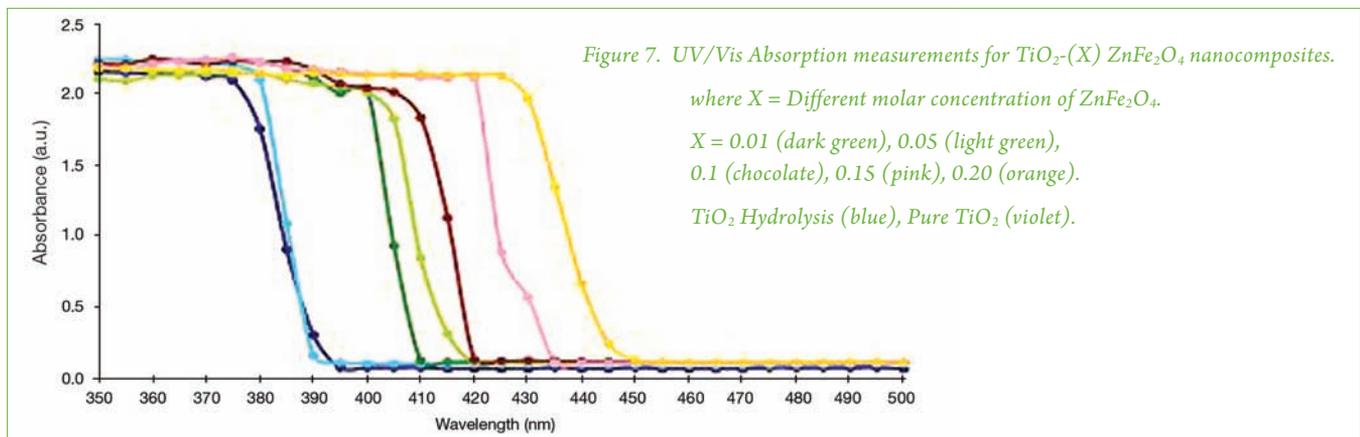


Figure 7. UV/Vis Absorption measurements for TiO<sub>2</sub>-(X) ZnFe<sub>2</sub>O<sub>4</sub> nanocomposites.

where X = Different molar concentration of ZnFe<sub>2</sub>O<sub>4</sub>.

X = 0.01 (dark green), 0.05 (light green), 0.1 (chocolate), 0.15 (pink), 0.20 (orange).

TiO<sub>2</sub> Hydrolysis (blue), Pure TiO<sub>2</sub> (violet).

## References

1. Hoffman, M., Martin, S., Choi, W., & Bahnemann, D. (1995). "Environmental applications of semiconductor photo catalysis," Chemical Review, vol. 95, pp. 69-96.
2. Wikipedia: Bandgap definition and diagram, <http://en.wikipedia.org/wiki/Bandgap>.
3. An Investigation of TiO<sub>2</sub>-ZnFe<sub>2</sub>O<sub>4</sub> Nanocomposites for Visible Light Photo catalysis by Jeremy Wade, A thesis submitted to Department of Electrical Engineering; College of Engineering, University of South Florida, March 24, 2005.
4. Fundamentals of Molecular Spectroscopy; C.N. Banwell University of Sussex, 3rd edition, May 1983.
5. Wikipedia: Effect of TiO<sub>2</sub> Nanoparticles on Polymer-Based Bulk Heterojunction Solar Cells  
<http://jjap.ipap.jp/link?JJAP/45/L1314/Bandgap>  
<http://www.ingentaconnect.com/content/els/02540584/2003/00000078/00000001/art00343>

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